**Fig. 2. Distribution of ΔG$^{off}$ for structures in different quality categories for all Targets.**
(A) Distributions of ΔG$^{off}$ from 1, 2 or 5 replicate MD simulations (left to right). Each set of ΔG$^{off}$ includes four bars which stand for high, medium, acceptable and incorrect structures respectively (left to right). (B) Direct comparison of the same quality category for ΔG$^{off}$ from 1, 2 or 5 replicates. Each quality category contains three bars: distribution from 1,2 and 5 replicates (left to right) . Note that Target 37 includes a JNK-interacting protein JIP4 which contain a leucine zipper domain (90 Å extended long coiled-coil) (Isabet et al., 2009). It needs huge amount of CPU-hours even with coarse-grained model and the result is only based on one replicate simulation. * Target 40 has two native interfaces (between chain AC and BC)